

10458286

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LOGINID:sssptal623hrr

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 SEP 01 New pricing for the Save Answers for SciFinder Wizard within
STN Express with Discover!
NEWS 4 OCT 28 KOREAPAT now available on STN
NEWS 5 NOV 30 PHAR reloaded with additional data
NEWS 6 DEC 01 LISA now available on STN
NEWS 7 DEC 09 12 databases to be removed from STN on December 31, 2004
NEWS 8 DEC 15 MEDLINE update schedule for December 2004
NEWS 9 DEC 17 ELCOM reloaded; updating to resume; current-awareness
alerts (SDIs) affected
NEWS 10 DEC 17 COMPUAB reloaded; updating to resume; current-awareness
alerts (SDIs) affected
NEWS 11 DEC 17 SOLIDSTATE reloaded; updating to resume; current-awareness
alerts (SDIs) affected
NEWS 12 DEC 17 CERAB reloaded; updating to resume; current-awareness
alerts (SDIs) affected
NEWS 13 DEC 17 THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS 14 DEC 30 EPFULL: New patent full text database to be available on STN
NEWS 15 DEC 30 CAPLUS - PATENT COVERAGE EXPANDED
NEWS 16 JAN 03 No connect-hour charges in EPFULL during January and
February 2005
NEWS 17 JAN 11 CA/CAPLUS - Expanded patent coverage to include Russia
(Federal Institute of Industrial Property)

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
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* * * * * STN Columbus * * * * *

10458286

FILE 'HOME' ENTERED AT 15:23:16 ON 25 JAN 2005

=> file registry

COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:23:26 ON 25 JAN 2005

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STRUCTURE FILE UPDATES: 23 JAN 2005 HIGHEST RN 819046-01-0

DICTIONARY FILE UPDATES: 23 JAN 2005 HIGHEST RN 819046-01-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

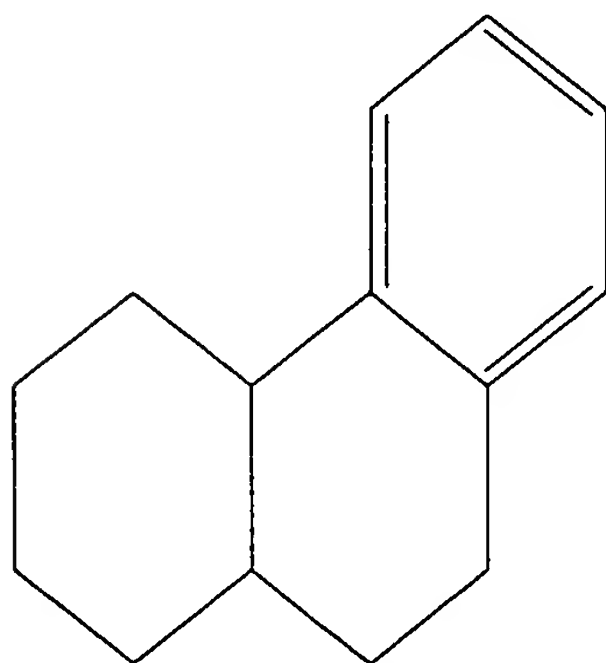
Uploading C:\STNEXP4\QUERIES\10664165-ring.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 15:23:49 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

< 23.0% PROCESSED 400000 ITERATIONS (1 INCOMPLETE) 33592 ANSWERS

10458286

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.09

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
 BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 144757

L2 33592 SEA SSS FUL L1

=> file caplus

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 161.33 | 161.54 |

FILE 'CAPLUS' ENTERED AT 15:24:07 ON 25 JAN 2005
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FILE COVERS 1907 - 25 Jan 2005 VOL 142 ISS 5
FILE LAST UPDATED: 24 Jan 2005 (20050124/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

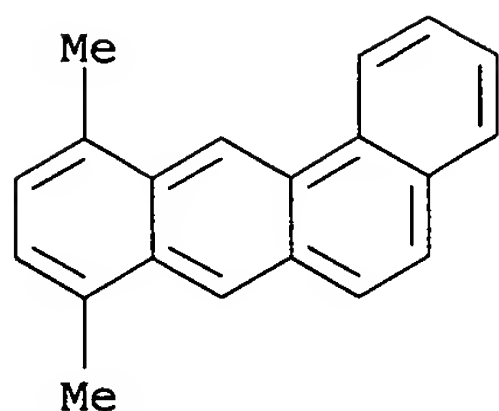
=> s l2

L3 5088 L2

=> d 5088 bib abs hitstr l3

L3 ANSWER 5088 OF 5088 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1913:20380 CAPLUS
DN 7:20380
OREF 7:2947e-i,2948a
TI Perylene and its Derivatives. II
AU Weitzenbock, Richard; Seer, Christian
CS Univ. Graz.
SO Ber. (1913), 46, 1994-2000
DT Journal
LA Unavailable
AB cf. C. A., 4, 2929.. (For nomenclature, see Bally and Scholl, C. A., 5, 3249). The yield of perylene can be increased to 4% by treating 1-C10H7Br with 3 parts of AlCl3 1 hr. at 140°. Under milder conditions (6 hrs. at 30-50°), from 20 g. C10H7Br were obtained traces of perylene; a small amount of a difficultly soluble substance, apparently a dinaphthyl naphthalene, C30H20, yellowish leaflets, m. 282-3°; and about 1 g. of 2,2'-binaphthyl, possibly formed by rearrangement of 1,1'-binaphthyl under the influence of the AlCl3. β-Dinaphthylene oxide, heated 1 hr. at 140° with 4 parts of AlCl3, gives about 6%

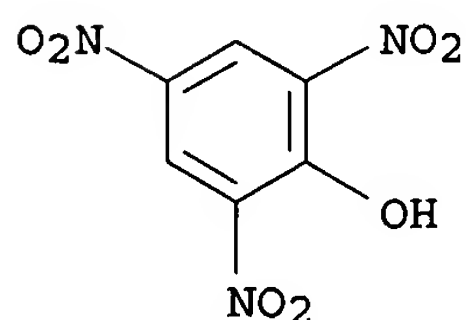
10458286



CM 2

CRN 88-89-1

CMF C6 H3 N3 O7



L3 ANSWER 5011 OF 5088 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1939:35193 CAPLUS
DN 33:35193
OREF 33:4981e-i,4982a-g
TI Syntheses in the phenanthrene series. II
AU Grewe, Rudolf
SO Ber. (1939), 72B, 785-90
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C. A. 33, 3782.4. Continuation of the work on the synthesis on 9,13-disubstituted phenanthrene derivs. in connection with the study of the structure of morphine alkaloids. In the present paper are reported some new observations which confirm the structure assigned to the α,β -unsatd. dicarboxylic acid (I) described in part I; furthermore, there have been obtained phenanthrene-9-carboxylic acids with an ang-Me group at position 13. I heated with freshly distilled quinoline and Naturkupfer C 2 hrs. at 200° is decarboxylated chiefly to 2-(β -phenyl- α -carboxyethyl)methylenecyclohexane, $\text{PhCH}_2\text{CH}(\text{CO}_2\text{H})\text{C}_6\text{H}_9\text{:CH}_2$ (II), m. 130°, and a smaller amount of an acid, m. 91° (probably formed from II by migration of the semicyclic double bond). Ozonolysis of II gave HCHO (isolated as the 2,4-dinitrophenylhydrazone (0.2 mol.), m. 162°), and the keto acid $\text{PhCH}_2\text{CH}(\text{CO}_2\text{H})\text{CH.CO.CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ (III), isolated as the semicarbazone (0.65 mol.) of the 174°-form of the Et ester. II undergoes ring closure with extraordinary ease, smoothly giving 2 compds. (IVa and IVb) which react with neither Br nor KMnO_4 and are ascribed the accompanying structure (in the original they are called 13-methyl-6,7,8,9,10,13,14-hexahydrophenanthrene-9-carboxylic acids but they are evidently the 5,6,7,8,9,10,13,14-octahydro compds.). On heating with Pd sponge up to 280°, which ordinarily dehydrogenates similar phenanthrene derivs. without an ang-Me group in a few min., they are hardly attacked, and only after long heating at about 320° could a small amount of an aromatic hydrocarbon, definitely identified as phenanthrene, be isolated. The

intermediate carboxylic acid is naturally at once decarboxylated at the temperature of the reaction. The recovered non-dehydrogenated material is always a mixture of IVa and IVb even when either of the pure isomers is used as starting material. None other of the total 4 possible racemates has thus far been obtained. Several attempts to effect complete aromatization of IVa and IVb with Se were unsuccessful. A vigorous reaction occurs but the crystalline products are not phenanthrenes; they form no addition product with

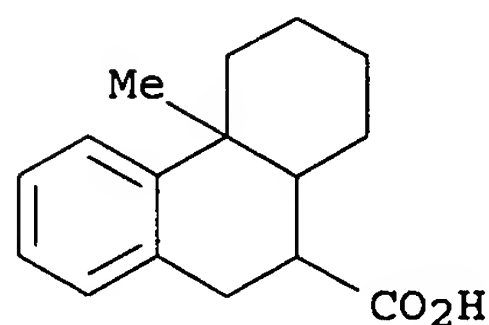
picric acid. A simplification of the synthesis of the IV by means of the Grignard reaction suggested itself. The ester of III can be converted with MeMgI into the lactone (V) only under definite conditions. During the reaction the primarily formed tertiary HO ester splits off EtOH. The yield is satisfactory and can be increased by starting directly from the free acid (III) and using 2 mols. MeMgI. By carefully working up the product it is possible to isolate the crystalline HO acid, PhCH₂CH(CO₂H)C₆H₉(OH)Me (VI), which, however, changes into V with extraordinary ease on gentle warming in ether. The lactone ring in V is only slowly opened by alkalies; it has thus far not been possible to prepare an ester of VI. The opening of the lactone ring is not necessary for the subsequent cyclization; with H₃PO₄ at 50°, V gives IVa and IVb with extraordinary ease. The striking ease of this rearrangement of V, which is so resistant toward other forms of attack, cannot be explained by the assumption alone of intermediate unsatd. acids. As V is easily soluble in cold H₃PO₄, probably phosphoric esters of HO acids of type VI have a decisive influence on the ring closure. V heated with P₂O₅ gives an entirely different result. There is formed a hydrocarbon C₁₅H₁₈ (VII), smoothly dehydrogenated to 1-methylphenanthrene, m. 119° (picrate, m. 135-6°) by heating with Pd. Since the Me group cannot have migrated under the mild conditions of the dehydrogenation, VII must have structure VIII or that of the Δ_{11,12}-isomer. The ultraviolet absorption spectrum, with maximum at 254 and 265 mμ, makes it probable that VII is a mixture of the 2 isomers. IVa and IVb, from II and sirupy H₃PO₄ at 80°, m. 142° and 178°, resp.

2-(β-Phenyl-α-carboxyethyl)-1-methylcyclohexanol (VI) (15 g. from 18 g. III in ether at 0° treated slowly with the Grignard reagent from 26 g. MeI, allowed to stand several hrs. at room temperature, heated some hrs. on the water bath and decomposed with much ice and dilute HCl), m. 121° (foaming). V (16 g. from 21 g. of the Et ester of III treated at 0° with the Grignard reagent from 8.5 cc. MeI in the course of several hrs., allowed to stand overnight at 0°, decomposed with ice and dilute HCl and, after evaporation of the ether, boiled 30 min. in 250 cc. alc. with 25 g. Girard reagent T and 25 cc. AcOH), b_{0.2} 167°. 1-Methylhexahydrophenanthrene (VII), b_{0.3} 124°.

IT 798557-11-6, 9-Phenanthrenecarboxylic acid, 4b,5,6,7,8,8a,9,10-octahydro-4b-methyl-
(isomers)

RN 798557-11-6 CAPLUS

CN 9-Phenanthrenecarboxylic acid, 4b,5,6,7,8,8a,9,10-octahydro-4b-methyl-
(4CI) (CA INDEX NAME)



10458286

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alerts (SDIs) affected
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NEWS 13 DEC 17 THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
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February 2005
NEWS 17 JAN 11 CA/CAPLUS - Expanded patent coverage to include Russia
(Federal Institute of Industrial Property)

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

NEWS HOURS STN Operating Hours Plus Help Desk Availability
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NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

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FILE 'HOME' ENTERED AT 15:23:16 ON 25 JAN 2005

=> file registry

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:23:26 ON 25 JAN 2005

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STRUCTURE FILE UPDATES: 23 JAN 2005 HIGHEST RN 819046-01-0

DICTIONARY FILE UPDATES: 23 JAN 2005 HIGHEST RN 819046-01-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

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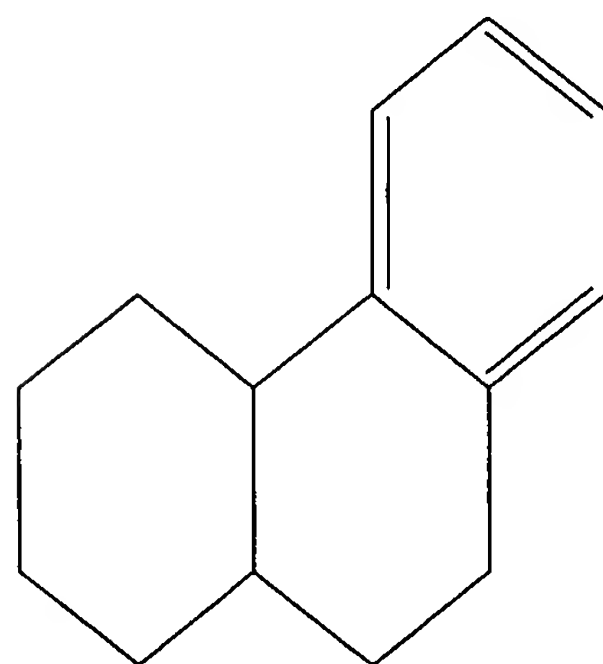
Uploading C:\STNEXP4\QUERIES\10664165-ring.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 15:23:49 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

< 23.0% PROCESSED 400000 ITERATIONS (1 INCOMPLETE) 33592 ANSWERS

10458286

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.09

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 144757

L2 33592 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 161.33 | 161.54 |

FULL ESTIMATED COST

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FILE COVERS 1907 - 25 Jan 2005 VOL 142 ISS 5
FILE LAST UPDATED: 24 Jan 2005 (20050124/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

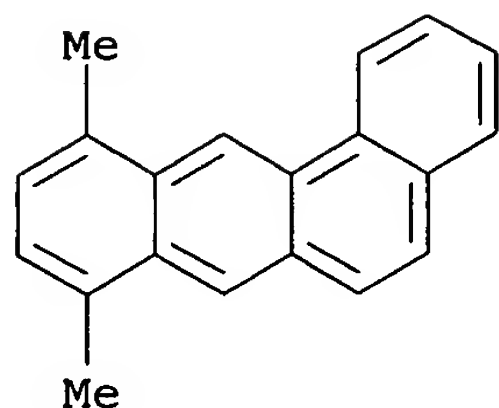
=> s 12

L3 5088 L2

=> d 5088 bib abs hitstr l3

L3 ANSWER 5088 OF 5088 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1913:20380 CAPLUS
DN 7:20380
OREF 7:2947e-i,2948a
TI Perylene and its Derivatives. II
AU Weitzenbock, Richard; Seer, Christian
CS Univ. Graz.
SO Ber. (1913), 46, 1994-2000
DT Journal
LA Unavailable
AB cf. C. A., 4, 2929.. (For nomenclature, see Bally and Scholl, C. A., 5, 3249). The yield of perylene can be increased to 4% by treating 1-C₁₀H₇Br with 3 parts of AlCl₃ 1 hr. at 140°. Under milder conditions (6 hrs. at 30-50°), from 20 g. C₁₀H₇Br were obtained traces of perylene; a small amount of a difficultly soluble substance, apparently a dinaphthyl naphthalene, C₃₀H₂₀, yellowish leaflets, m. 282-3°; and about 1 g. of 2,2'-binaphthyl, possibly formed by rearrangement of 1,1'-binaphthyl under the influence of the AlCl₃. β-Dinaphthylene oxide, heated 1 hr. at 140° with 4 parts of AlCl₃, gives about 6%

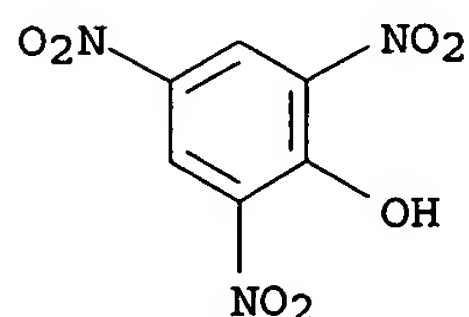
10458286



CM 2

CRN 88-89-1

CMF C6 H3 N3 O7



L3 ANSWER 5011 OF 5088 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1939:35193 CAPLUS
DN 33:35193
OREF 33:4981e-i,4982a-g
TI Syntheses in the phenanthrene series. II
AU Grewe, Rudolf
SO Ber. (1939), 72B, 785-90
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C. A. 33, 3782.4. Continuation of the work on the synthesis on 9,13-disubstituted phenanthrene derivs. in connection with the study of the structure of morphine alkaloids. In the present paper are reported some new observations which confirm the structure assigned to the α,β -unsatd. dicarboxylic acid (I) described in part I; furthermore, there have been obtained phenanthrene-9-carboxylic acids with an ang-Me group at position 13. I heated with freshly distilled quinoline and Naturkupfer C 2 hrs. at 200° is decarboxylated chiefly to 2-(β -phenyl- α -carboxyethyl)methylenecyclohexane, $\text{PhCH}_2\text{CH}(\text{CO}_2\text{H})\text{C}_6\text{H}_9\text{:CH}_2$ (II), m. 130°, and a smaller amount of an acid, m. 91° (probably formed from II by migration of the semicyclic double bond). Ozonolysis of II gave HCHO (isolated as the 2,4-dinitrophenylhydrazone (0.2 mol.), m. 162°), and the keto acid $\text{PhCH}_2\text{CH}(\text{CO}_2\text{H})\text{CH.CO.CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ (III), isolated as the semicarbazone (0.65 mol.) of the 174°-form of the Et ester. II undergoes ring closure with extraordinary ease, smoothly giving 2 compds. (IVa and IVb) which react with neither Br nor KMnO_4 and are ascribed the accompanying structure (in the original they are called 13-methyl-6,7,8,9,10,13,14-hexahydrophenanthrene-9-carboxylic acids but they are evidently the 5,6,7,8,9,10,13,14-octahydro compds.). On heating with Pd sponge up to 280°, which ordinarily dehydrogenates similar phenanthrene derivs. without an ang-Me group in a few min., they are hardly attacked, and only after long heating at about 320° could a small amount of an aromatic hydrocarbon, definitely identified as phenanthrene, be isolated. The

intermediate carboxylic acid is naturally at once decarboxylated at the temperature of the reaction. The recovered non-dehydrogenated material is always a mixture of IVa and IVb even when either of the pure isomers is used as starting material. None other of the total 4 possible racemates has thus far been obtained. Several attempts to effect complete aromatization of IVa and IVb with Se were unsuccessful. A vigorous reaction occurs but the crystalline products are not phenanthrenes; they form no addition product with

picric acid. A simplification of the synthesis of the IV by means of the Grignard reaction suggested itself. The ester of III can be converted with MeMgI into the lactone (V) only under definite conditions. During the reaction the primarily formed tertiary HO ester splits off EtOH. The yield is satisfactory and can be increased by starting directly from the free acid (III) and using 2 mols. MeMgI. By carefully working up the product it is possible to isolate the crystalline HO acid, PhCH₂CH(CO₂H)C₆H₉(OH)Me (VI), which, however, changes into V with extraordinary ease on gentle warming in ether. The lactone ring in V is only slowly opened by alkalies; it has thus far not been possible to prepare an ester of VI. The opening of the lactone ring is not necessary for the subsequent cyclization; with H₃PO₄ at 50°, V gives IVa and IVb with extraordinary ease. The striking ease of this rearrangement of V, which is so resistant toward other forms of attack, cannot be explained by the assumption alone of intermediate unsatd. acids. As V is easily soluble in cold H₃PO₄, probably phosphoric esters of HO acids of type VI have a decisive influence on the ring closure. V heated with P₂O₅ gives an entirely different result. There is formed a hydrocarbon C₁₅H₁₈ (VII), smoothly dehydrogenated to 1-methylphenanthrene, m. 119° (picrate, m. 135-6°) by heating with Pd. Since the Me group cannot have migrated under the mild conditions of the dehydrogenation, VII must have structure VIII or that of the Δ^{11,12}-isomer. The ultraviolet absorption spectrum, with maximum at 254 and 265 mμ, makes it probable that VII is a mixture of the 2 isomers. IVa and IVb, from II and sirupy H₃PO₄ at 80°, m. 142° and 178°, resp.

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IT 798557-11-6, 9-Phenanthrenecarboxylic acid, 4b,5,6,7,8,8a,9,10-octahydro-4b-methyl-
(isomers)

RN 798557-11-6 CAPLUS

CN 9-Phenanthrenecarboxylic acid, 4b,5,6,7,8,8a,9,10-octahydro-4b-methyl-
(4CI) (CA INDEX NAME)

